

A Level Set Approach to Optimal Homogenized Coefficients

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Abstract: The reconstructing optimal microstructures of given homogenized coefficients of steady diffusion equation is studied. In the reconstruction, the governing equation of level set function is approximated by adding viscosity term and the numerical procedure for the evolution of the level set function for the solution is examined. The numerical experiments of reconstruction are obtained by applying a finite element method with locally fitted mesh.

keyword: Homogenization, level set, reconstruction, locally fitted mesh

1 Introduction

Composite materials consist of two or more different materials, in microscopic scale, usually assumed to have periodic structures. However, such composite materials in microscopic scale are not of interest when they are actually used. Instead, the (effective) material properties in macroscopic scale, which is measured by usual tools, are more often useful. The theory and technique of homogenization are the realization of the effective material properties in macroscopic scale from the microscopic structures of composite materials. The main topic of the paper is to optimally design microscopic structures of composite materials to give certain macroscopic material properties.

The notion of the set of all effective moduli of two different mixtures has been well investigated by introducing G_θ sets. See Allaire and Kohn (1993); Bendsoe and Soares (1993); Bendsoe (1995); Suzuki and Kikuchi (1991) and the references therein, for the problem of optimal topology design of composite materials. Suzuki and Kikuchi (1991), for example, approximated G_θ set in microscopically square shape and Haslinger and Dvořák

(1995) extended to star-shaped microstructures, using standard minimization algorithms.

In this paper, the level set method for finding optimal microstructures for given effective conductivity to the diffusion is studied. Since the topology of the optimal microstructure is not known, it is necessary to handle the moving and splitting of the interface of the two mixtures. The level set method overcomes these difficulties easily. The evolution of level set function is calculated by finite element methods in this paper while the evolution has been studied by applying the finite element method designed in Osher and Sethian (1988). Also, the finite element mesh is locally fitted for the microstructure which is also used in calculating the effective moduli (conductivity) by homogenization. The paper is organized as follows. In Section 2, the cost function and admissible set are introduced and the existence of the solution is presented. In Section 3, we calculate the derivatives of homogenized coefficients which are used to obtain the velocity of the level set functions. In Section 4, the level set approach is introduced. In Section 5, we give the locally fitted mesh procedure which is done for each iterated level set function, and give figures which show the success of attainment of optimal microstructure whose topology is different from that of initial guess.

2 Construction of optimal microstructures

For simplicity, we consider only for the homogenized coefficients or the effective conductivities, each phase of which is isotropic, that is,

$$a_{ij}(y) = a_D(y)\delta_{ij} \quad \text{where}$$

$$a_D(y) = \begin{cases} \alpha, & y \in D, \\ \beta, & y \in Y \setminus D, \end{cases} \quad (2.1)$$

for $y \in Y$, $\xi \in \mathbf{R}^2$, $Y \equiv [0, 1] \times [0, 1]$ and D is a measurable subset included in Y (See **Fig. 2**). As the conditions for α, β , it is assumed that there exists a real number $\gamma > 0$ such that

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$$a_{ij}(y)\xi_i\xi_j \geq \gamma\xi_i\xi_i, \quad y \in Y, \quad \xi \in \mathbf{R}^2. \quad (2.2)$$

Set $\Gamma = \partial\Omega$ and consider the following boundary value problem for linear conductivity equation

$$-\nabla \cdot (a^\varepsilon(x)\nabla u^\varepsilon(x)) = f(x), \quad \text{in } \Omega, \quad (2.3a)$$

$$u^\varepsilon(x) = 0, \quad \text{on } \partial\Omega. \quad (2.3b)$$

Here, the parameter ε is a positive real number and $\Omega \subseteq \mathbf{R}^2$, $\partial\Omega$ is a Lipschitz boundary and $a^\varepsilon(x) = a(x/\varepsilon)$ with the function $a(\cdot)$ being extended onto \mathbf{R}^2 periodically with period Y . The periodic medium represented by $a^\varepsilon(x)$ is shown in Fig. 1.

It is well known by homogenization theory, for instance, as described in Hornung (1997); Sanchez-Palencia (1980), that $u^\varepsilon \rightharpoonup u^0$ weakly in $H^1(\Omega)$ as $\varepsilon \rightarrow 0$, where $u^0 \in H^1(\Omega)$ is the solution of

$$-\frac{\partial}{\partial x_i} \left(a_{ij}^* \frac{\partial u^0}{\partial x_j} \right) = f \quad \text{in } \Omega, \quad (2.4)$$

$$u^0 = 0 \quad \text{on } \partial\Omega.$$

For the first equation of (2.4), the homogenized coefficients or the effective conductivities a_{ij}^* are given by

$$a_{ij}^* = \int_Y a_D(y) \left(\delta_{ij} - \frac{\partial \omega^{(j)}}{\partial y_i}(y) \right) dy, \quad (2.5)$$

where $\omega^{(j)} \in H_{per}^1(Y)$ is the solution of

$$\int_Y a_D(y) \nabla \omega^{(j)} \cdot \nabla \varphi dy = \int_Y a_D(y) \frac{\partial \varphi}{\partial y_j} dy, \quad \varphi \in H_{per}^1(Y). \quad (2.6)$$

Since the solution of (2.6) is unique up to an additive constant, we impose an extra condition on their representatives so that the mean value of $\omega^{(j)}$ vanishes. From now on, $\dot{H}_{per}^1(Y)$ is denoted as the subspace of $H_{per}^1(Y)$ with mean zero.

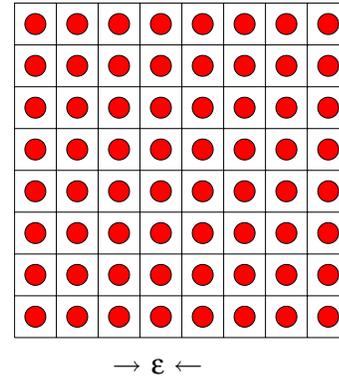


Fig. 1. Periodic medium in coordinate x .

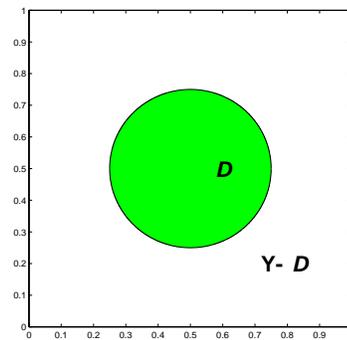


Fig. 2. Standard microcell in coordinate y .

For the equation (2.5), we see that the homogenized coefficients a_{ij}^* depend on a_D which indicates the microstructure. The microstructure represents how two different materials are mixed. Let $a^*(a_D)$ be the homogenized coefficient from the microscopic configuration determined by a_D . We are interested in optimizing the microscopic structure to reproduce the homogenized coefficient \bar{a} which is in G_θ .

In this paper, a level set method is proposed for constructing more general microstructures for the matrices (or moduli) in G_θ than star-shaped, single inclusion geometries parametrized by a polar function around the center of Y on which Haslinger and Dvořák (1995) worked.

In order to get the optimal shape of given effective material constants, we minimize the following cost function

$$K(D) = K(a^*(a_D)) = \frac{1}{2} \sum_{ij} (a_{ij}^*(a_D) - \bar{a}_{ij})^2, \quad (2.7)$$

for the microscopic configuration D . Thus our problem

is formulated as the following minimization problem :

$$(P) \quad \text{Find the minimizer } \bar{D} \in \vartheta \\ \text{such that } K(\bar{D}) = \min_{D \in \vartheta} K(D),$$

where $K(D) = K(a^*(a_D))$ and ϑ is an admissible set. To ensure the existence of a solution of (P), the following condition for the admissible set is necessary:

$$\text{For any } \{D_n\}_{n \rightarrow \infty} \subseteq \vartheta, \text{ there exist a subsequence } \\ \{D_{n'}\} \subseteq \{D_n\} \text{ and } D \in \vartheta \text{ such that} \quad (2.8) \\ \chi_{D_{n'}} \rightarrow \chi_D \text{ in } L^2(Y),$$

where χ_E denotes the characteristic function of a set $E \subset Y$. It is known that (see for example Bendsoe (1995); Sokolowski and Zolesio (1992)) the following ϑ satisfies (2.8) :

$$\vartheta \equiv \{D \subset Y \mid \text{per}(D) \leq M\}, \quad (2.9)$$

where M is a fixed constant and

$$\text{per}(D) \equiv \sup \left\{ \int_D \nabla \cdot \varphi \, dy \mid \varphi \in C_0^1(Y, \mathbf{R}^2), \right. \\ \left. \|\varphi\|_{L^\infty(Y)} \leq 1 \right\}.$$

Indeed, we have

Proposition 2.1 *Let Y be a bounded domain in \mathbf{R}^n . For any $M > 0$, the set ϑ in (2.9) is compact in $L^2(Y)$ in the sense of (2.8).*

Proof. See De Giorgi, Colombini, and Pinccini (1972).

The choice of the admissible set (2.9) means restricting the possible range of material sets to measurable sets of bounded perimeter, i.e. the total length of the boundaries of the structure is constrained.

Remark 2.2 *Another admissible set $\tilde{\vartheta}$ is also used widely, which is the set of subdomains D which satisfies the following two conditions;*

1. $\bar{A} \subseteq D \subseteq \bar{B}$ for some A, B which are nonempty subdomains of Y .
2. There exists $\bar{\varepsilon} > 0$ such that for any $D \in \tilde{\vartheta}$ possesses the $\bar{\varepsilon}$ -cone property given in Grisvard (1985).

This choice of $\tilde{\vartheta}$ satisfies the condition (2.8). The admissible set $\tilde{\vartheta}$ preserves the regularity of boundary of domain, while the admissible set ϑ in (2.9) does not preserve the regularity.

To ensure the existence of solution to minimization problem (P), the lower semicontinuity of K is necessary. From now on, the symbol $D_n \rightarrow D$ as $n \rightarrow \infty$ is used to denote the convergence of domains in the sense that

$$\chi(D_n) \rightarrow \chi(D) \text{ in } L^2(Y) \text{ as } n \rightarrow \infty.$$

The lower semicontinuity of K is equivalent to

$$\text{if } D_n \rightarrow D, \text{ then } K(D) \leq \liminf_{n \rightarrow \infty} K(D_n), \quad (2.10)$$

which is guaranteed by the following lemma with a proof given in Haslinger and Dvořák (1995);

Lemma 2.3 (Continuity) *Let $D_n \rightarrow D$, where $D_n, D \in \vartheta$. Then we have*

$$a_{ij}^*(a_{D_n}) \rightarrow a_{ij}^*(a_D) \quad \text{as } n \rightarrow \infty.$$

Thus we have

Theorem 2.4 (Existence) *There exists at least one solution of (P).*

Proof. The proof can be obtained by a standard method, see e.g. Struwe (1990).

3 Derivatives of homogenized coefficients

This section is devoted to finding Jacobian matrix $J_{a^*}(a_D)(\delta a_D)$, whose components are derivatives of homogenized coefficients. For a real number $s > 0$, let $\omega_s^{(j)}$ and $\omega^{(j)} \in \dot{H}_{\text{per}}^1(Y)$ be the solutions of the following equations,

$$\int_Y (a_D + s\delta a_D) \nabla \omega_s^{(j)} \cdot \nabla v \, dy = \int_Y (a_D + s\delta a_D) \frac{\partial v}{\partial y_j} \, dy, \\ \int_Y a_D \nabla \omega^{(j)} \cdot \nabla v \, dy = \int_Y a_D \frac{\partial v}{\partial y_j} \, dy, \quad (3.1)$$

respectively, where $v \in H_{\text{per}}^1(Y)$. Let $\hat{\omega}^{(j)} \in \dot{H}_{\text{per}}^1(Y)$ be the solution of

$$\int_Y a_D \nabla \hat{\omega}^{(j)} \cdot \nabla v \, dy = \int_Y \delta a_D \frac{\partial v}{\partial y_j} \, dy \\ - \int_Y \delta a_D \nabla \omega^{(j)} \cdot \nabla v \, dy, \quad (3.2)$$

for $v \in H^1_{per}(Y)$. Define $z_s^{(j)}$ as

$$z_s^{(j)} \equiv \frac{\omega_s^{(j)} - \omega^{(j)}}{s}. \tag{3.3}$$

Lemma 3.1 *If $\delta a_D \in L^\infty(Y)$, then $z_s^{(j)} \rightarrow \dot{\omega}^{(j)}$ strongly in $H^1_{per}(Y)$ as $s \rightarrow 0$.*

Proof. By subtracting the second equation from the first of (3.1), we have

$$\begin{aligned} \int_Y s\delta a_D \nabla \omega_s^{(j)} \cdot \nabla v \, dy + \int_Y a_D (\nabla \omega_s^{(j)} - \nabla \omega^{(j)}) \cdot \nabla v \, dy \\ = \int_Y s\delta a_D \frac{\partial v}{\partial y_j} \, dy. \end{aligned}$$

Thus $z_s^{(j)}$ in (3.3) is the solution of

$$\int_Y a_D \nabla z_s^{(j)} \cdot \nabla v \, dy = \int_Y \delta a_D \frac{\partial v}{\partial y_j} \, dy - \int_Y \delta a_D \nabla \omega_s^{(j)} \cdot \nabla v \, dy. \tag{3.4}$$

Since $\omega_s^{(j)}$ and $\omega^{(j)} \in \dot{H}^1_{per}(Y)$, the function $z_s^{(j)}$ is in $\dot{H}^1_{per}(Y)$. Then, by putting $v = z_s^{(j)}$, we have

$$\begin{aligned} \gamma \int_Y |\nabla z_s^{(j)}|^2 \, dy &\leq \int_Y a_D |\nabla z_s^{(j)}|^2 \, dy \\ &= \int_Y \delta a_D e_j \cdot \nabla z_s^{(j)} \, dy - \int_Y \delta a_D \nabla \omega_s^{(j)} \cdot \nabla z_s^{(j)} \, dy \\ &\leq M \left\{ \left(\int_Y |e_j|^2 \, dy \right)^{1/2} + \left(\int_Y |\nabla \omega_s^{(j)}|^2 \, dy \right)^{1/2} \right\} \\ &\quad \left(\int_Y |\nabla z_s^{(j)}|^2 \, dy \right)^{1/2}, \end{aligned}$$

where $e_j = y_j$, $M = \|\delta a_D\|_\infty$ and γ is given in (2.2). Similarly, by putting $v = \omega_s^{(j)}$ in (3.1) we have for sufficiently small s

$$\begin{aligned} \widehat{\gamma} \int_Y |\nabla \omega_s^{(j)}|^2 \, dy &\leq \int_Y (a_D + s\delta a_D) \nabla \omega_s^{(j)} \cdot \nabla \omega_s^{(j)} \, dy \\ &= \int_Y (a_D + s\delta a_D) e_j \cdot \nabla \omega_s^{(j)} \, dy \\ &\leq \left(\int_Y |a_D + s\delta a_D|^2 \, dy \right)^{1/2} \\ &\quad \left(\int_Y |\nabla \omega_s^{(j)}|^2 \, dy \right)^{1/2}, \end{aligned} \tag{3.5}$$

where $\widehat{\gamma}$ is taken so that

$$\widehat{\gamma} \leq \gamma/2.$$

Since if $0 < \alpha \leq \beta$, then $|a_D + s\delta a_D| < 2\beta$ in Y for sufficiently small s , $\omega_s^{(j)}$ is bounded in $\dot{H}^1_{per}(Y)$ independently of s , and hence $z_s^{(j)}$ is bounded in $\dot{H}^1_{per}(Y)$ independently of s . Thus there exist a subsequence, still denoted by $\{z_s^{(j)}\}$, and $z_0^{(j)} \in \dot{H}^1_{per}(Y)$ such that

$$z_s^{(j)} \rightharpoonup z_0^{(j)} \text{ in } \dot{H}^1_{per}(Y) \text{ as } s \rightarrow 0.$$

Since $z_0^{(j)}$ satisfies the equation (3.2) and by the uniqueness of the solution for a weakly formulated elliptic problem in $\dot{H}^1_{per}(Y)$, we have

$$z_0^{(j)} = \dot{\omega}^{(j)}, \quad j = 1, 2.$$

For the strong convergence of $\{z_s^{(j)}\}$ to $\dot{\omega}^{(j)}$, subtract (3.4) from (3.2). Then we have

$$\begin{aligned} \int_Y a_D (\nabla \dot{\omega}^{(j)} - \nabla z_s^{(j)}) \cdot \nabla v \, dy \\ = - \int_Y \delta a_D (\nabla \omega^{(j)} - \nabla \omega_s^{(j)}) \cdot \nabla v \, dy. \end{aligned}$$

Let $v = \dot{\omega}^{(j)} - z_s^{(j)}$. Then

$$\begin{aligned} \gamma \int_Y |\nabla (\dot{\omega}^{(j)} - z_s^{(j)})|^2 \, dy \\ \leq \int_Y a_D |\nabla (\dot{\omega}^{(j)} - z_s^{(j)})|^2 \, dy \\ = - \int_Y \delta a_D \nabla (\omega^{(j)} - \omega_s^{(j)}) \cdot \nabla (\dot{\omega}^{(j)} - z_s^{(j)}) \, dy \\ \leq M \left(\int_Y |\nabla (\omega^{(j)} - \omega_s^{(j)})|^2 \, dy \right)^{1/2} \\ \quad \left(\int_Y |\nabla (\dot{\omega}^{(j)} - z_s^{(j)})|^2 \, dy \right)^{1/2}, \end{aligned}$$

where $M = \|\delta a_D\|_\infty$. Since $\|z_s^{(j)}\|_{\dot{H}^1_{per}(Y)}$ is bounded independently of s , we know that

$$\int_Y |\nabla (\omega^{(j)} - \omega_s^{(j)})|^2 \, dy \rightarrow 0 \text{ as } s \rightarrow 0.$$

Thus we conclude that

$$z_s^{(j)} \rightarrow \dot{\omega}^{(j)} \text{ in } \dot{H}^1_{per}(Y) \text{ as } s \rightarrow 0. \tag{3.6}$$

Theorem 3.2 *Let $\delta a_D \in L^\infty(Y)$. Then the derivatives of homogenized coefficients, $J_{a^*}(a_D)$ are represented as*

$$\begin{aligned} (J_{a^*}(a_D)(\delta a_D))_{ij} = \int_Y \delta a_D \left[\delta_{ij} - \frac{\partial \omega^{(i)}}{\partial y_j} - \frac{\partial \omega^{(j)}}{\partial y_i} \right. \\ \left. + \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} \right] \, dy, \quad i, j = 1, 2. \end{aligned}$$

Proof. Notice that (2.5) can be rewritten by using (2.6) given by as

$$a_{ij}^*(a_D) = \int_Y a_D \delta_{ij} dy - \int_Y a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy.$$

Thus we get

$$\begin{aligned} a_{ij}^*(a_D + s\delta a_D) &= \int_Y (a_D + s\delta a_D) \delta_{ij} dy \\ &\quad - \int_Y (a_D + s\delta a_D) \nabla \omega_s^{(i)} \cdot \nabla \omega_s^{(j)} dy, \\ a_{ij}^*(a_D) &= \int_Y a_D \delta_{ij} dy - \int_Y a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy. \end{aligned}$$

By subtracting $a_{ij}^*(a_D)$ from $a_{ij}^*(a_D + s\delta a_D)$, we have

$$\begin{aligned} a_{ij}^*(a_D + s\delta a_D) - a_{ij}^*(a_D) &= \int_Y s\delta a_D \delta_{ij} dy \\ &\quad - \int_Y (a_D + s\delta a_D dy - a_D) \nabla \omega_s^{(i)} \cdot \nabla \omega_s^{(j)} dy \\ &\quad - \int_Y a_D (\nabla \omega_s^{(i)} - \nabla \omega^{(i)}) \cdot \nabla \omega_s^{(j)} dy \\ &\quad - \int_Y a_D \nabla \omega^{(i)} \cdot (\nabla \omega_s^{(j)} - \nabla \omega^{(j)}) dy. \end{aligned}$$

Hence, by Lemma 3.1, we have

$$\begin{aligned} \lim_{s \rightarrow 0} \frac{a_{ij}^*(a_D + s\delta a_D) - a_{ij}^*(a_D)}{s} &= \\ &\int_Y \delta a_D \delta_{ij} dy - \int_Y \delta a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy \\ &\quad - \int_Y a_D \nabla \dot{\omega}^{(i)} \cdot \nabla \omega^{(j)} dy - \int_Y a_D \nabla \omega^{(i)} \cdot \nabla \dot{\omega}^{(j)} dy. \end{aligned}$$

Put $v = \omega^{(i)}$ in (3.2). Then,

$$\begin{aligned} \int_Y a_D \nabla \dot{\omega}^{(j)} \cdot \nabla \omega^{(i)} dy &= \int_Y \delta a_D \frac{\partial \omega^{(i)}}{\partial y_j} dy \\ &\quad - \int_Y \delta a_D \nabla \omega^{(j)} \cdot \nabla \omega^{(i)} dy. \end{aligned}$$

Similarly, we have

$$\begin{aligned} \int_Y a_D \nabla \dot{\omega}^{(i)} \cdot \nabla \omega^{(j)} dy &= \int_Y \delta a_D \frac{\partial \omega^{(j)}}{\partial y_i} dy \\ &\quad - \int_Y \delta a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy. \end{aligned}$$

Thus $J_{a^*}(a_D)$, which are the Jacobian of $a^*(a_D)$, are

$$\begin{aligned} (J_{a^*}(a_D)(\delta a_D))_{ij} &\equiv \lim_{s \rightarrow 0} \frac{a_{ij}^*(a_D + s\delta a_D) - a_{ij}^*(a_D)}{s} \\ &= \int_Y \delta a_D \delta_{ij} dy - \int_Y \delta a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy \\ &\quad - \left(\int_Y \delta a_D \frac{\partial \omega^{(i)}}{\partial y_j} dy - \int_Y \delta a_D \nabla \omega^{(j)} \cdot \nabla \omega^{(i)} dy \right) \\ &\quad - \left(\int_Y \delta a_D \frac{\partial \omega^{(j)}}{\partial y_i} dy - \int_Y \delta a_D \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} dy \right) \\ &= \int_Y \delta a_D \left[\delta_{ij} - \frac{\partial \omega^{(i)}}{\partial y_j} - \frac{\partial \omega^{(j)}}{\partial y_i} + \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} \right] dy. \end{aligned}$$

For the formal adjoint of J_{a^*} , note that

$$\begin{aligned} \int_Y \delta a_D J_{a^*}(a_D)^T(p) dy &= \langle p, J_{a^*}(a_D)(\delta a_D) \rangle \\ &= \sum_{i,j=1}^2 p_{ij} \int_Y \delta a_D \\ &\quad \left[\delta_{ij} - \frac{\partial \omega^{(i)}}{\partial y_j} - \frac{\partial \omega^{(j)}}{\partial y_i} + \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} \right] dy \\ &= \int_Y \delta a_D \sum_{i,j=1}^2 p_{ij} \\ &\quad \left[\delta_{ij} - \frac{\partial \omega^{(i)}}{\partial y_j} - \frac{\partial \omega^{(j)}}{\partial y_i} + \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} \right] dy, \end{aligned}$$

for a second order tensors p where $\langle \cdot, \cdot \rangle$ denotes the inner product in \mathbf{R}^4 . Thus we obtain

$$\begin{aligned} J_{a^*}(a_D)^T(p) &= \sum_{i,j=1}^2 p_{ij} \\ &\quad \left[\delta_{ij} - \frac{\partial \omega^{(i)}}{\partial y_j} - \frac{\partial \omega^{(j)}}{\partial y_i} + \nabla \omega^{(i)} \cdot \nabla \omega^{(j)} \right]. \end{aligned}$$

4 The level set approach

The level set methods have been developed for the description of the motion of curves and surfaces by Osher and Sethian (1988).

In the level set methods, the given curves or surfaces are interpreted as zero level set of ϕ , a smooth level set function defined in the domain containing the physical domain where the curves or the surfaces evolve. Hence a curve (or a surface) can develop corners, cusp, and

undergo topological changes as the level set function evolves. For the level set formulation, consider a closed $(N - 1)$ -dimensional hypersurface $\Gamma(t = 0)$ which propagates along its normal direction with speed V , where V is a function of the curvature, normal direction and others. Let $\phi(x, 0)$, where $x \in \mathbf{R}^n$, be the signed distance function from x to $\Gamma(t = 0)$, defined by

$$\phi(x, 0) = \phi_0 \equiv \pm d(x, \Gamma(t = 0)), \tag{4.1}$$

where the plus(minus) sign indicates if x is outside(inside) the initial hypersurface $\Gamma(t = 0)$. Thus the relation between $\Gamma(0)$ and $\phi(x, 0)$ is:

$$\Gamma(t = 0) = \{x \mid \phi(x, 0) = 0\}.$$

What we are going to do is to get the equation for the level set function $\phi(x, t)$ which evolves such that

$$\Gamma(t) = \{x \mid \phi(x, t) = 0\}. \tag{4.2}$$

Let $x(t)$ be the path of a point on the propagation front. Then $x_t \cdot n = V(x(t))$ with the vector x_t normal to the front at $x(t)$. Since (4.2) must be satisfied, we have

$$\phi(x(t), t) = 0. \tag{4.3}$$

By the chain rule, we have

$$\phi_t + \nabla\phi(x(t), t) \cdot x_t(t) = 0.$$

Since $n = \nabla\phi/|\nabla\phi|$ and $x_t(t) \cdot n = V(x, t)$, we have the formulation

$$\begin{cases} \phi_t + V|\nabla\phi| &= 0, \\ \phi(x, 0) &= \phi_0(x). \end{cases} \tag{4.4}$$

More detailed contents can be found in Chang, Hou, Merriman, and Osher (1996); Malladi, Sethian, and Vemuri (1995); Osher and Sethian (1988); Sethian (1996); Sussman, Smereka, and Osher (1994); Zhu and Sethian (1992). Santosa (1996) used the level set method for an obstacle reconstruction problem. In the same way, we apply the method to obtain the optimal microstructures of composite of two different mixtures for given effective conductivity.

Let $\{D_n\}$ be the minimizing sequence of the cost function K in (2.7) and let D_n, D_{n+1} be characterized by the functions ϕ_n, ϕ_{n+1} such that

$$D_n = \{y \mid \phi_n(y) \leq 0\}, \tag{4.5}$$

$$D_{n+1} = \{y \mid \phi_{n+1}(y) \leq 0\}. \tag{4.6}$$

Here D_0 denote the initial guess of microgeometry of the region of α .

Thus finding D_{n+1} from D_n corresponds to finding ϕ_{n+1} from ϕ_n . Consider the following equation;

$$\begin{cases} \phi_t + V(y, t)|\nabla\phi| = 0 & \text{for } (y, t) \in Y \times (t_n, t_{n+1}], \\ \phi(y, t_n) = \widehat{\phi}_n(y) & \text{for } y \in Y, \end{cases} \tag{4.7}$$

where $\widehat{\phi}_n$ is the signed distance function reinitialized from the zero level set of ϕ_n .

Let $\phi_{n+1}(y)$ denote the function $\phi(y, t_n)$. Then it is necessary to find such $V(y, t)$.

Concerning the choice of $V(y, t)$, we follow Santosa (1996), in spite of the lack of the theoretical basis :

$$\begin{aligned} V(y, t) &= -\text{sign}(\alpha - \beta)(J_{a^*})^T(a^* - \bar{a}) \\ &= -\text{sign}(\alpha - \beta) \left(\sum_{ij} \left[\delta_{ij} - \frac{\partial\omega^{(i)}}{\partial y_j} - \frac{\partial\omega^{(j)}}{\partial y_i} \right. \right. \\ &\quad \left. \left. + \nabla\omega^{(i)} \cdot \nabla\omega^{(j)} \right] (a^*(a_D) - \bar{a})_{ij} \right), \end{aligned} \tag{4.8}$$

to obtain D_{n+1} such that $K(D_{n+1}) < K(D_n)$.

Remark 4.1 If $\omega^{(i)}$ and $\omega^{(j)}$ belong to $H^s(Y)$ for $2 < s$, these are embedded into $C^{1-q}, 0 < q < 1$ (page 35 of Grisvard (1985)). Thus there is no theoretical lack. However, $\omega^{(i)}$ and $\omega^{(j)}$ belong to $H^s(Y)$ for $1 < s < 3/2$, thus the trace of

$$\delta_{ij} - \frac{\partial\omega^{(i)}}{\partial y_j} - \frac{\partial\omega^{(j)}}{\partial y_i} + \nabla\omega^{(i)} \cdot \nabla\omega^{(j)}$$

is not well-defined.

5 Numerical examples

Since the classical solution of (4.4) is not available beyond a certain time or is not determined uniquely, it is necessary to introduce a weak solution called a viscosity solution.

Definition 5.1 A viscosity subsolution(supersolution) of (4.4) is a function $u \in C(\Omega \times [0, T])$ for all $T > 0$ such that for all $\phi \in C^1(\Omega \times (0, \infty))$, if (x_0, t_0) is a local maximum(minimum) point of $(u - \phi)$ on $\Omega \times (0, T)$, then

$$\frac{\partial\phi}{\partial t}(x_0, t_0) + V(x_0, t_0)|\nabla\phi(x_0, t_0)| \leq (\geq) 0.$$

A function u is called a viscosity solution if u is a viscosity sub and supersolution.

Two approximations of the solution of (4.4) are proposed in Crandall and Lions (1984). One is the finite difference approximation and the other an approximation with viscosity term, so called the method of vanishing viscosity. Here, we use the viscosity term to approximate (4.4). We consider the following periodic initial boundary value problem

$$\begin{aligned} \phi_t^\varepsilon - \varepsilon \Delta \phi^\varepsilon + V(y, t) |\nabla \phi^\varepsilon| &= 0 \quad \text{for } (y, t) \in Y \times [0, T], \\ \text{periodic boundary condition on } \partial Y \times [0, T], \\ \phi^\varepsilon(y, 0) &= \phi_0(y), \end{aligned} \tag{5.1}$$

where $\varepsilon > 0$, $T > 0$ and $Y = [0, 1] \times [0, 1]$. In the numerical test, the finite element method to initial-boundary value problem (5.1) is used for the level set method instead of Osher and Sethian's scheme. The finite element mesh is locally fitted for the microstructures. For the locally fitting procedure, we follow the idea given in Börgers (1990).

5.1 The locally fitting procedure

Consider a rectangular grid $\widehat{\Xi}$ covering $Y = [0, 1] \times [0, 1]$. Denote the grid points by

$$\widehat{\mathbf{x}}_{ij} = (\widehat{x}_i, \widehat{y}_j) = ((i-1)h, (j-1)h), \quad 1 \leq i \leq M, \quad 1 \leq j \leq N,$$

where, for convenience, $M = N$ and h is the mesh grid size. We also use notation $\mathbf{x} = (x, y) \in Y$. Note the level set function ϕ gives the mapping

$$\phi : \widehat{\Xi} \rightarrow \mathbf{R}$$

such that

$$\phi = \begin{cases} \leq 0 & \text{if } \widehat{\mathbf{x}} \in D, \\ > 0 & \text{if } \widehat{\mathbf{x}} \in Y \setminus D. \end{cases}$$

Let us find the zero points of ϕ as follows.

For $i = 1, \dots, M$:

For $j = 1, \dots, N-1$:

$$\text{If } \phi(\widehat{\mathbf{x}}_{ij}) \cdot \phi(\widehat{\mathbf{x}}_{i(j+1)}) < 0$$

Determine $y \in [(j-1)h, jh]$ with $\phi((i-1)h, y) = 0$, and mark

$$\begin{cases} \widehat{\mathbf{x}}_{i(j+1)} & \text{if } y \geq (j - \frac{1}{2})h \\ \widehat{\mathbf{x}}_{ij} & \text{otherwise} \end{cases}$$

End of j .

End of i .

For $j = 1, \dots, N$:

For $i = 1, \dots, M-1$:

$$\text{If } \phi(\widehat{\mathbf{x}}_{ij}) \cdot \phi(\widehat{\mathbf{x}}_{(i+1)j}) < 0$$

Determine $x \in [(i-1)h, ih]$ with $\phi(x, (j-1)h) = 0$, and mark

$$\begin{cases} \widehat{\mathbf{x}}_{(i+1)j} & \text{if } x \geq (i - \frac{1}{2})h \\ \widehat{\mathbf{x}}_{ij} & \text{otherwise} \end{cases}$$

End for i .

End for j .

Perturb $\widehat{\Xi}$ by moving the marked points near the boundary ∂D onto ∂D . This results in an almost rectangular grid Ξ , whose points are denoted by

$$\mathbf{x}_{ij} = (x_i, y_j), \quad 1 \leq i \leq M, \quad 1 \leq j \leq N.$$

Let us define

$$I \equiv \{\mathbf{x} \in \Xi \mid \phi(\mathbf{x}) < 0\},$$

$$B \equiv \{\mathbf{x} \in \Xi \mid \phi(\mathbf{x}) = 0\},$$

$$E \equiv \{\mathbf{x} \in \Xi \mid \phi(\mathbf{x}) > 0\}.$$

The points in I, B and E are called the interior, boundary and exterior points, respectively. Then

$$\Xi = I \cup B \cup E.$$

Note that the values of ϕ at the nodes on ∂D are all zero. Let \widehat{B} be the set of the points of $\widehat{\Xi}$ which corresponds to B of Ξ . Thus

$$\widehat{\Xi} = I \cup \widehat{B} \cup E.$$

Let Q be the quadrilateral with vertices $\mathbf{x}_{ij}, \mathbf{x}_{i,j+1}, \mathbf{x}_{i+1,j}$ and $\mathbf{x}_{i+1,j+1}$. Let d_1, d_2 be the two diagonals of Q . We assign μ_l to d_l , for $l = 1, 2$, as follows

$$(Q, d_l) \rightarrow \mu_l \equiv \min_{k=1,2} \frac{\det D\psi(k)(d_l)}{\lambda_{\max}((D\psi(k)(d_l))^T (D\psi(k)(d_l)))},$$

where $\lambda_{\max}(\cdot)$ denotes the larger of the two eigenvalues and $\psi(k)(d_l)$ is the affine mapping from $\hat{\tau}_k(d_l)$ to $\tau_k(d_l)$. $\tau_k(d_l)$, $k = 1, 2$, are the resulting triangles by d_l and $\hat{\tau}_k(d_l)$, $k = 1, 2$, are the corresponding triangles in $\hat{\Xi}$ for $l = 1, 2$. Since the larger μ_l is, the less degenerate is the configuration resulted from cutting Q along d_l ,

if $\mu_1 \geq \mu_2$, then choose d_1 ,
 else, choose d_2 .

By measuring μ , we decide along which to cut the quadrilateral cells Q of the grid Ξ . The details are referred to Börgers (1990). In Fig. 3 and Fig 4, we show the microstructure and the corresponding locally fitted mesh, respectively.

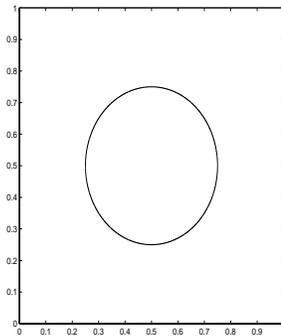


Fig. 3. Microstructure of circle type.

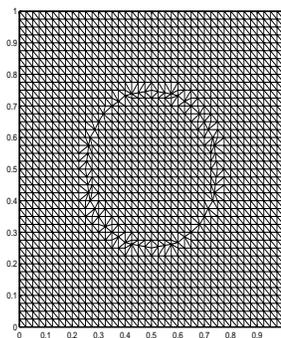


Fig. 4. Locally fitted mesh for circle.

$a_{12} = 0.0$, $a_{21} = 0.0$ and $a_{22} = 1.5$. The viscosity coefficient ϵ is taken as 0.001. The underlying finite element mesh is 41×41 . The following table shows the history of the iteration of our level set method.

Table 1. Iteration history of the optimality

iteration	K	a_{11}	a_{12}	a_{22}
1	0.21364	1.3606	0.0053	1.3646
2	0.10217	1.5684	-0.0742	1.5842
3	0.0576	1.8380	-0.0653	1.7836
4	0.025397	1.9042	-0.0545	1.6889
5	0.019929	1.8470	-0.0569	1.5998
11	0.0018156	1.9638	-0.0073	1.5470
51	0.0012152	1.9632	-0.0048	1.5321
91	0.00058364	1.9664	-0.0014	1.4941
101	9.6545e-05	1.9916	-0.0011	1.5109
118	2.7756e-15	2.0000	0.0000	1.5000

In the following series of figures, the left hand sides represent the level set function and the right hand sides the corresponding microstructure. In the figures of microstructures, the darker regions represents D and the lighter regions $Y \setminus D$.

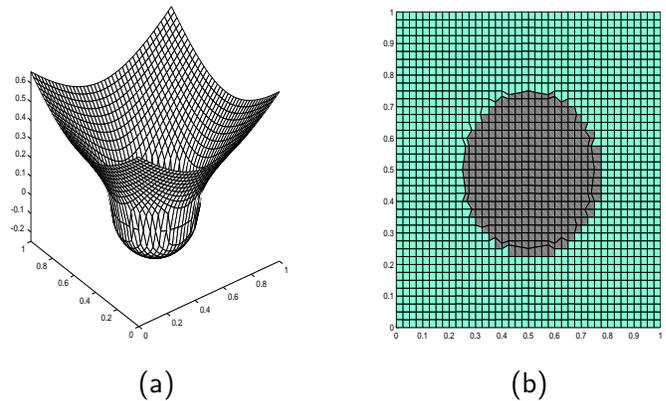


Fig. 5. (a) shows the first level set function and (b) shows the corresponding first microstructure with cost 0.21364.

5.2 Numerical examples

We show a numerical example. It is chosen that $\alpha = 3, \beta = 1$. The initial microstructure is given such that D is the circle with center at $(0.5, 0.5)$ and the radius 0.25, which is the nonpositive region of $\text{sign}((y_1 - 0.5)^2 + (y_2 - 0.5)^2 - 0.25^2) \sqrt{(y_1 - 0.5)^2 + (y_2 - 0.5)^2 - 0.25^2}$ and $Y \setminus D$ is the outside of the circle (See Fig. 5(b)). The target homogenized coefficients are given by $a_{11} = 2.0$,

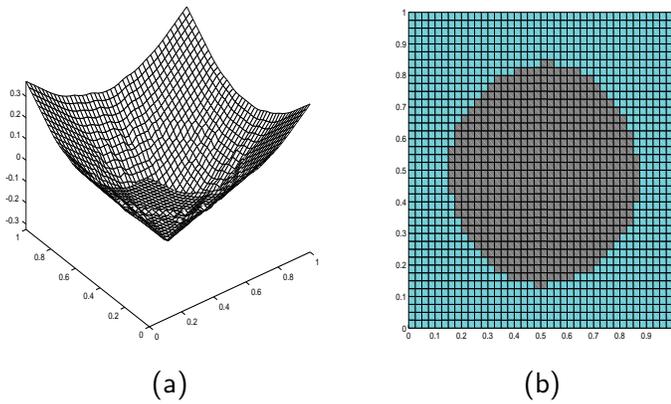


Fig. 6. (a) shows the second level set function and (b) shows the corresponding second microrstructure with cost 0.10217.

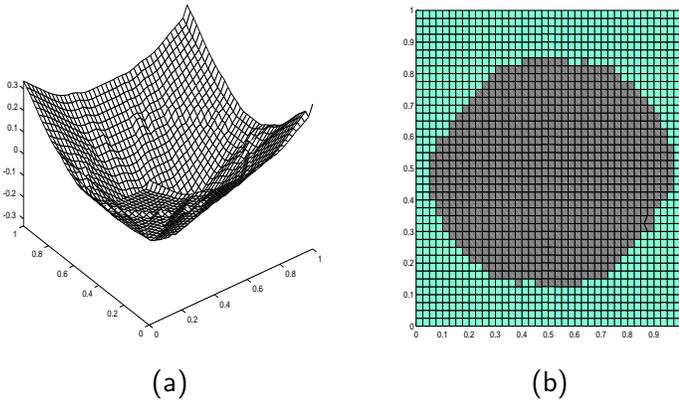


Fig. 7. (a) shows the third level set function and (b) shows the corresponding third microrstructure with cost 0.0576.

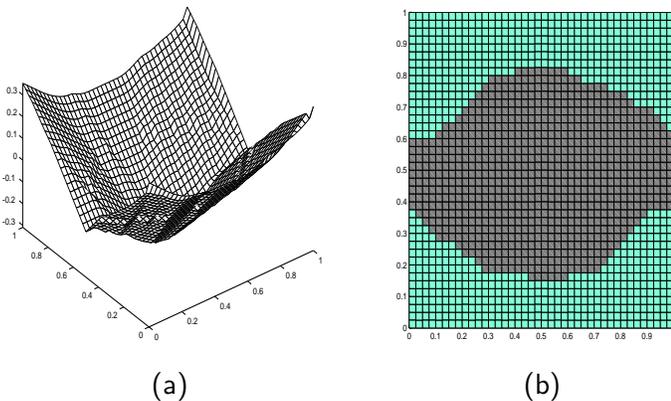


Fig. 8. (a) shows the fourth level set function and (b) shows the corresponding fourth microrstructure with cost 0.025397.

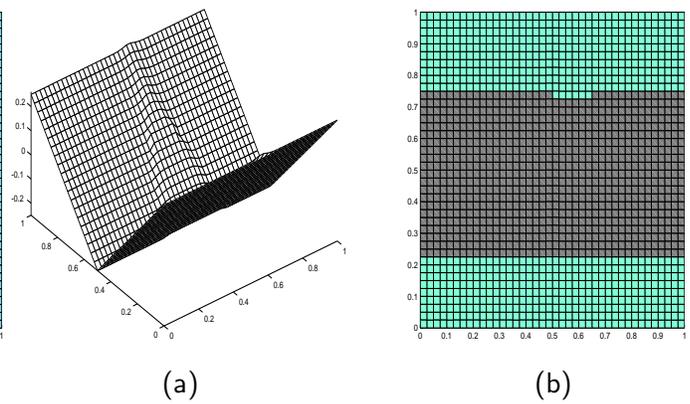


Fig. 9. (a) shows the 101-st level set function and (b) shows the corresponding 101-st microrstructure with cost $9.6545e-05$.

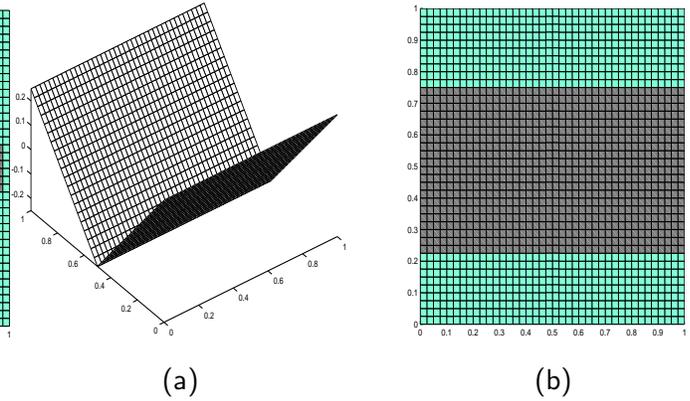


Fig. 10. (a) shows the 118-th level set function and (b) shows the corresponding 118-th microrstructure with cost $2.7756e-15$.

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